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Radiative Transport Equation for Bloch Electrons in Electromagnetic Fields

Received: date / Accepted: date

Abstract The radiative transport equation for the Schrödinger equation in a periodic potential with a weak random potential in electromagnetic fields is derived using asymptotic expansion.

Keywords Radiative transport · Waves in random media · Bloch waves

1 Introduction

The radiative transport equation (RTE) is a linear Boltzmann equation, which describes propagation of energy density in a random medium [1, 2]. Rigorous analysis on the transport limit for the Schrödinger equation with random potential has been studied [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. In particular, the RTE was obtained from the Schrödinger equation with time independent [10] and time dependent [11] random potential. In [12], the RTE was derived from the Schrödinger equation with random and periodic potential. See also recent review [13] and references therein. In the absence of random potential, the semiclassical equations of motion for the Schrödinger equation with periodic potential and electromagnetic fields has been considered [14, 15, 16, 17, 18, 19].

In this paper, we consider noninteracting electrons in a periodic potential (Bloch electrons) with a weak random potential and apply electromagnetic fields. For this system, the RTE is derived in the same way as [12] except that we here take electromagnetic fields into account.

This paper is organized as follows. In Sec. 2, a two-scale asymptotic expansion is introduced for the Wigner distribution function. In Sec. 3, Bloch functions are considered. The Wigner distribution function is decomposed in Sec. 4 and Sec. 5

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making use of the Bloch functions. Finally, we derive the RTE and obtain our main result Eq. (79) in Sec. 6.

2 The Schrödinger Equation

We consider Bloch electrons in an electric field $E \in R^3$ and a magnetic field $B \in R^3$. They are given by vector potential $A \in R^3$ and scalar potential $\varphi \in R$ as

$$E = -\nabla\varphi - \frac{\partial}{\partial t}A, \quad B = \nabla \times A. \quad (1)$$

The state $\psi(t, x) \in R$ ($t \in R, x \in R^3$) of this system evolves according to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(t, x) = \mathcal{H} \psi(t, x). \quad (2)$$

The Hamiltonian \mathcal{H} is given as

$$\mathcal{H} = \frac{1}{2m_e} (p + eA)^2 + e\varphi + U_{\text{tot}}(x), \quad (3)$$

where $p = -i\hbar\nabla_x$, $-e$ and m_e are the charge and mass of an electron, and $U_{\text{tot}}(x) = U(x) + V(x)$. Here $U(x)$ is a d -dimensional ($d \leq 3$) periodic potential and $V(x)$ is a random potential. The periodic potential satisfies

$$U(z + v) = U(z), \quad (4)$$

where v belongs to the lattice L :

$$L = \left\{ \sum_{j=1}^d n_j e_j \mid n_j \in Z \right\} \quad (5)$$

and e_1, \dots, e_d form a basis of R^d with the dual basis e^1, \dots, e^d defined by $e_j \cdot e^k = 2\pi\delta_{jk}$. The dual lattice L^* is spanned by $\{e^k\}$. We let C denote the basic period cell of L and Ω_{BZ} denote the Brillouin zone. Note that

$$|C|\Omega_{\text{BZ}} = (2\pi)^d. \quad (6)$$

The random potential has the following properties.

$$\langle V(y)V(y+x) \rangle = R(x), \quad \langle \tilde{V}(q)\tilde{V}(q') \rangle = (2\pi)^d \tilde{R}(q') \delta(q+q'). \quad (7)$$

Here $\langle \cdot \rangle$ denotes ensemble average and the Fourier transform is defined as

$$\tilde{V}(q) = \int_{R^d} dx e^{-iq \cdot x} V(x). \quad (8)$$

Because of the $U(1)$ gauge symmetry, we can set

$$\varphi = 0. \quad (9)$$

We scale the variables as

$$t \rightarrow \frac{t}{\varepsilon}, \quad x \rightarrow \frac{x}{\varepsilon}, \quad (10)$$

where $\varepsilon (> 0)$ is small. We assume weak electromagnetic fields:

$$E \rightarrow \varepsilon E, \quad B \rightarrow \varepsilon B. \quad (11)$$

Equation (1) implies that A is independent of ε . Since the cyclotron radius ℓ is inversely proportional to $|B|$, we have $\ell \rightarrow \ell/\varepsilon$ and ℓ gets much larger than the cell size of the lattice L . Furthermore, we assume that the random potential is weak. We obtain

$$\begin{aligned} \frac{\partial}{\partial t} \psi_\varepsilon(t, x) &= \frac{i\hbar\varepsilon}{2m_e} \left[\nabla_x + \frac{ie}{\hbar\varepsilon} A(t, x) \right]^2 \psi_\varepsilon(t, x) + \frac{1}{i\hbar\varepsilon} U\left(\frac{x}{\varepsilon}\right) \psi_\varepsilon(t, x) \\ &\quad + \frac{1}{i\hbar\sqrt{\varepsilon}} V\left(\frac{x}{\varepsilon}\right) \psi_\varepsilon(t, x), \end{aligned} \quad (12)$$

where the initial wave function $\psi_\varepsilon(0, x) \in L^2(R^d)$ is ε -oscillatory. In [12], the RTE is derived from this equation in the absence of the vector potential $A(t, x)$.

Let us consider the Wigner distribution function associated with ψ_ε .

$$W_\varepsilon(t, x, k) = \int_{R^d} \frac{dy}{(2\pi)^d} e^{ik \cdot y} \psi_\varepsilon(t, x - \varepsilon y) \bar{\psi}_\varepsilon(t, x). \quad (13)$$

Whenever necessary, we use the fact that $k \in R^d$ is uniquely decomposed as

$$k = q + \mu, \quad q \in \Omega_{\text{BZ}}, \quad \mu \in L^*. \quad (14)$$

Note that $W_\varepsilon(t, x, k)$ and its symmetric version

$$\int_{R^d} \frac{dy}{(2\pi)^d} e^{ik \cdot y} \psi_\varepsilon\left(t, x - \frac{\varepsilon}{2}y\right) \bar{\psi}_\varepsilon\left(t, x + \frac{\varepsilon}{2}y\right) \quad (15)$$

have the same weak limit as $\varepsilon \rightarrow 0$ [20]. We obtain the time evolution of W_ε as

$$\begin{aligned} \frac{\partial}{\partial t} W_\varepsilon(t, x, k) &+ \left[\frac{\hbar k}{m_e} \cdot \nabla_x + \frac{i\hbar\varepsilon}{2m_e} \Delta_x + \frac{e}{m_e} \left(A(t, x) \cdot \nabla_x - k \cdot A(t, \nabla_\mu) \right) \right. \\ &\quad \left. - \frac{e^2}{m_e \hbar} \left(A(t, x) + \frac{i\varepsilon}{2} A(t, \nabla_\mu) \right) \cdot A(t, \nabla_\mu) \right] W_\varepsilon(t, x, k) \\ &= \frac{1}{i\hbar\varepsilon} \sum_{\mu' \in L^*} e^{i\mu' \cdot x/\varepsilon} \tilde{U}(\mu') [W_\varepsilon(t, x, k - \mu') - W_\varepsilon(t, x, k)] \\ &\quad + \frac{1}{i\hbar\sqrt{\varepsilon}} \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot x/\varepsilon} \tilde{V}(k') [W_\varepsilon(t, x, k - k') - W_\varepsilon(t, x, k)], \end{aligned} \quad (16)$$

where we used

$$\psi_\varepsilon(t, x) \frac{\partial}{\partial x_j} \psi_\varepsilon(t, x) \xrightarrow{x_j \rightarrow \infty} 0, \quad (j = 1, \dots, d), \quad (17)$$

and introduced

$$U(y) = \sum_{\mu \in L^*} e^{i\mu \cdot y} \tilde{U}(\mu), \quad \tilde{U}(\mu) = \frac{1}{|C|} \int_C dy e^{-i\mu \cdot y} U(y). \quad (18)$$

Note that we have

$$\frac{1}{|C|} \sum_{\mu \in L^*} e^{i\mu \cdot z} = \sum_{v \in L} \delta(z - v). \quad (19)$$

Let us define

$$H(x, \mu, q) = \frac{\hbar}{2m_e} \left[k + \frac{e}{\hbar} A(t, x) \right]^2. \quad (20)$$

Noting that

$$\frac{\partial A(x)}{\partial x_i} \frac{\partial}{\partial \mu_i} = A(t(0, \dots, 0, \frac{\partial}{\partial \mu_i}, 0, \dots, 0)), \quad (21)$$

we obtain

$$\begin{aligned} \frac{\partial}{\partial t} W_\varepsilon + [\nabla_\mu H(x, \mu, q) \cdot \nabla_x - \nabla_x H(x, \mu, q) \cdot \nabla_\mu] W_\varepsilon(t, x, k) = \\ \left[-\frac{i\hbar\varepsilon}{2m_e} \Delta_x + \frac{i\varepsilon e^2}{2m_e \hbar} A(t, \nabla_\mu) \cdot A(t, \nabla_\mu) \right] W_\varepsilon(t, x, k) \\ + \frac{1}{i\hbar\varepsilon} \sum_{\mu' \in L^*} e^{i\mu' \cdot x/\varepsilon} \tilde{U}(\mu') [W_\varepsilon(t, x, k - \mu') - W_\varepsilon(t, x, k)] \\ + \frac{1}{i\hbar\sqrt{\varepsilon}} \int_{\mathbb{R}^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot x/\varepsilon} \tilde{V}(k') [W_\varepsilon(t, x, k - k') - W_\varepsilon(t, x, k)]. \end{aligned} \quad (22)$$

We note that the term $-\nabla_x H$ is responsible for the Lorentz force:

$$\begin{aligned} -\nabla_x H &= -\frac{e}{m_e} \nabla_x (k \cdot A) + O(|A|^2), \\ -\frac{e}{m_e} \nabla_x (k \cdot A) &= -\frac{e}{m_e} [(k \cdot \nabla_x) A + k \times (\nabla_x \times A)] \\ &= -\frac{e}{\hbar} [-E + v \times B], \end{aligned} \quad (23)$$

where $\hbar k = m_e v + eA$ and $v = dx/dt$. The left-hand side of Eq. (22) can be expressed as

$$\frac{\partial}{\partial t} W_\varepsilon + \left[H\left(x - \frac{1}{2} \nabla_\mu, \mu + \frac{1}{2} \nabla_x, q\right) - H\left(x + \frac{1}{2} \nabla_\mu, \mu - \frac{1}{2} \nabla_x, q\right) \right] W_\varepsilon(t, x, k). \quad (24)$$

This expression was first obtained by Kubo [21].

We introduce a two-scale expansion for W_ε :

$$W_\varepsilon(t, x, k) = W_0(t, x, z, k) + \sqrt{\varepsilon} W_1(t, x, z, k) + \varepsilon W_2(t, x, z, k) + \dots \quad (25)$$

We assume that W_0 is deterministic and periodic with respect to $z = x/\varepsilon$. We replace

$$\nabla_x \rightarrow \nabla_x + \frac{1}{\varepsilon} \nabla_z. \quad (26)$$

By collecting terms of $O(\varepsilon^{-1})$, we have

$$\mathcal{L}W_0 = 0, \quad (27)$$

where the skew symmetric operator \mathcal{L} is given by

$$\begin{aligned} \mathcal{L}f(z, k) &= \nabla_\mu H(x, \mu, q) \cdot \nabla_z f(z, k) + \frac{i\hbar}{2m_e} \Delta_z f(z, k) \\ &\quad - \frac{1}{i\hbar} \sum_{\mu' \in L^*} e^{i\mu' \cdot z} \tilde{U}(\mu') [f(z, k - \mu') - f(z, k)] \\ &= \left[\frac{\hbar k}{m_e} + \frac{e}{m_e} A(t, x) \right] \cdot \nabla_z f(z, k) + \frac{i\hbar}{2m_e} \Delta_z f(z, k) \\ &\quad - \frac{1}{i\hbar} \sum_{\mu' \in L^*} e^{i\mu' \cdot z} \tilde{U}(\mu') [f(z, k - \mu') - f(z, k)]. \end{aligned} \quad (28)$$

By collecting terms of $O(\varepsilon^{-1/2})$, we have

$$\mathcal{L}W_1 = \frac{1}{i\hbar} \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \tilde{V}(k') [W_0(t, x, k - k') - W_0(t, x, k)]. \quad (29)$$

By collecting terms of $O(1)$, we have

$$\begin{aligned} \frac{\partial}{\partial t} W_0 + (\nabla_\mu H \cdot \nabla_x - \nabla_x H \cdot \nabla_\mu) W_0 &= -\mathcal{L}W_2 - \frac{i\hbar}{m_e} \nabla_x \cdot \nabla_z W_0(t, x, k) \\ &\quad + \frac{1}{i\hbar} \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \tilde{V}(k') [W_1(t, x, k - k') - W_1(t, x, k)]. \end{aligned} \quad (30)$$

3 The Bloch Functions

To obtain the eigenvalues and eigenfunctions of the operator \mathcal{L} , we consider the following eigenproblem.

$$\left[\frac{1}{2m_e} \left(\frac{\hbar}{i} \nabla_z + eA(t, x) \right)^2 + U(z) \right] \Phi_{m\alpha}(z, q) = E_m(q) \Phi_{m\alpha}(z, q). \quad (31)$$

Here, α labels degenerate energy levels of E_m with multiplicity r_m : $\alpha = 1, \dots, r_m$. We assume that there is no level crossing and

$$E_1(q) \leq E_2(q) \leq \dots. \quad (32)$$

The parameter $q \in R^d$ labels eigenvalues of the translational operator T ($= e^{v \cdot \nabla_z}$, $v \in L$):

$$T\Phi(z, q) = \Phi(z + v, q) = e^{iq \cdot v} \Phi(z, q). \quad (33)$$

Note that q moves inside the Brillouin zone (Ω_{BZ}). It is, however, convenient to extend $\Phi(z, q)$ to R^d in q with L^* -periodic. The eigenfunctions $\Phi_{m\alpha}(z, q)$ form a complete orthonormal basis in $L^2(C)$:

$$(\Phi_{m\alpha}, \Phi_{j\beta}) = \int_C \frac{dz}{|C|} \Phi_{m\alpha}(z, q) \bar{\Phi}_{j\beta}(z, q) = \delta_{mj} \delta_{\alpha\beta}. \quad (34)$$

We rewrite the eigenproblem using the periodic function

$$\phi(z, q) = e^{-iq \cdot z} \Phi(z, q). \quad (35)$$

We obtain

$$\left[\frac{1}{2m_e} \left(\frac{\hbar}{i} \nabla_z + \hbar q + eA(t, x) \right)^2 + U(z) \right] \phi_{m\alpha}(z, q) = E_m(q) \phi_{m\alpha}(z, q). \quad (36)$$

By differentiating the equation with respect to q_j , we obtain

$$\frac{\partial E_m}{\partial q_j} \delta_{mn} \delta_{\alpha\beta} = -i \frac{\hbar^2}{m_e} \left(\frac{\partial \phi_{m\alpha}}{\partial z_j}, \phi_{n\beta} \right) + \frac{\hbar^2}{m_e} \left(q_j + \frac{e}{\hbar} A_j \right) \delta_{mn} \delta_{\alpha\beta}. \quad (37)$$

Thus we have

$$\frac{\partial E_m}{\partial q_j} \delta_{mn} \delta_{\alpha\beta} = -i \frac{\hbar^2}{m_e} \left(\frac{\partial \Phi_{m\alpha}}{\partial z_j}, \Phi_{n\beta} \right) + \frac{e\hbar}{m_e} A_j(t, x) \delta_{mn} \delta_{\alpha\beta}. \quad (38)$$

Similarly, we also have

$$\left(A_l \frac{\partial \Phi_{m\alpha}}{\partial z_j}, \Phi_{n\beta} \right) = \frac{im_e}{\hbar^2} \frac{\partial E_m}{\partial q_j} (A_l \Phi_{m\alpha}, \Phi_{n\beta}) - \frac{ie}{\hbar} A_j(t, x) (A_l \Phi_{m\alpha}, \Phi_{n\beta}), \quad (39)$$

where

$$(A_l \Phi_{m\alpha}, \Phi_{n\beta}) = \int_C \frac{dz}{|C|} A_l(t, z) \Phi_{m\alpha}(z, q) \bar{\Phi}_{n\beta}(z, q). \quad (40)$$

The Bloch functions satisfy the following orthogonality relations [12].

$$\frac{1}{\Omega_{\text{BZ}}} \sum_{m, \alpha} \int_{\text{BZ}} dq \Phi_{m\alpha}(x, q) \bar{\Phi}_{m\alpha}(y, q) = \delta(y - x), \quad (41)$$

$$\frac{1}{\Omega_{\text{BZ}}} \int_{\mathbb{R}^d} dx \Phi_{j\alpha}(x, q) \bar{\Phi}_{m\beta}(x, q') = \delta_{jm} \delta_{\alpha\beta} \delta(q - q'). \quad (42)$$

4 Decomposition of W_0

Let us define the z -periodic functions $Q_{mn}^{\alpha\beta}(z, \mu, q)$, $\mu \in L^*$, $q \in \Omega_{\text{BZ}}$ by

$$Q_{mn}^{\alpha\beta}(z, \mu, q) = \int_C \frac{dy}{|C|} e^{i(q+\mu) \cdot y} \Phi_{m\alpha}(z - y, q) \bar{\Phi}_{n\beta}(z, q). \quad (43)$$

These functions satisfy the following orthogonality relation.

$$\sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) Q_m^{\alpha'\beta'}(z, \mu, q) = \delta_{jm} \delta_{\alpha\alpha'} \delta_{\beta\beta'}. \quad (44)$$

They are eigenfunctions of \mathcal{L} :

$$\mathcal{L} Q_{mn}^{\alpha\beta}(z, \mu, q) = \frac{i}{\hbar} [E_m(q) - E_n(q)] Q_{mn}^{\alpha\beta}(z, \mu, q), \quad (45)$$

with $k = q + \mu$.

Let us write $Q_{mm}^{\alpha\beta}$ as $Q_m^{\alpha\beta}$. Equation (45) implies that $\ker \mathcal{L}$ is spanned by $Q_m^{\alpha\beta}$. By Eq. (27), $W_0(t, x, z, k)$ may be decomposed as

$$W_0(t, x, z, k) = W_0(t, x, z, q + \mu) = \sum_{m, \alpha, \beta} \{u_m(t, x, q)\}_{\alpha\beta} Q_m^{\alpha\beta}(z, \mu, q), \quad (46)$$

where $u_m(t, x, q)$ is a $r_m \times r_m$ matrix.

5 Decomposition of W_1

Let us look at Eq. (29). In general, W_1 is not periodic in the fast variable z . Hence, instead of $Q_{mn}^{\alpha\beta}$, we use the basis functions

$$P_{mn}^{\alpha\beta}(z, \mu, q, q_0) = \int_C \frac{dy}{|C|} e^{i(q+\mu) \cdot y} \Phi_{m\alpha}(z - y, q) \bar{\Phi}_{n\beta}(z, q + q_0), \quad (47)$$

where $z \in R^d$ and $q, q_0 \in \Omega_{\text{BZ}}$. The functions $P_{mn}^{\alpha\beta}$ are quasi-periodic in z :

$$P_{mn}^{\alpha\beta}(z + v, \mu, q, q_0) = P_{mn}^{\alpha\beta}(z, \mu, q, q_0) e^{-iv \cdot q_0}, \quad (48)$$

where $v \in L$. Using Eq. (19), Eq. (34), and Eq. (42), we obtain the following orthogonality relation.

$$\sum_{\mu \in L^*} \int_{R^d} \frac{dz}{\Omega_{\text{BZ}}} P_{mn}^{\alpha\beta}(z, \mu, q, q') \bar{P}_{jl}^{\alpha'\beta'}(z, \mu, q, q'') = \delta_{mj} \delta_{nl} \delta_{\alpha\alpha'} \delta_{\beta\beta'} \delta(q' - q''). \quad (49)$$

The functions $P_{mn}^{\alpha\beta}$ are also eigenfunctions of \mathcal{L} .

$$\mathcal{L} P_{mn}^{\alpha\beta}(z, \mu, q, q_0) = \frac{i}{\hbar} [E_m(q) - E_n(q + q_0)] P_{mn}^{\alpha\beta}(z, \mu, q, q_0). \quad (50)$$

We write W_1 in this basis as

$$W_1(t, x, z, q + \mu) = \sum_{mn\alpha\beta} \int_{\text{BZ}} \frac{dq'}{\Omega_{\text{BZ}}} \eta_{mn}^{\alpha\beta}(t, x, q, q') P_{mn}^{\alpha\beta}(z, \mu, q, q'), \quad (51)$$

where $z \in R^d$, $q \in \Omega_{\text{BZ}}$, and $\mu \in L^*$. We plug this into Eq. (29), multiply $\bar{P}_{jl}^{\alpha\beta}(z, \mu, q, q_0)$, sum over $\mu \in L^*$, and integrate over $z \in R^d$. The lhs becomes

$$\begin{aligned} \sum_{\mu \in L^*} \int_{R^d} dz \bar{P}_{jl}^{\alpha\beta}(z, \mu, q, q_0) \mathcal{L} \sum_{mn\alpha'\beta'} \int_{\text{BZ}} \frac{dq'}{\Omega_{\text{BZ}}} \eta_{mn}^{\alpha'\beta'}(t, x, q, q') P_{mn}^{\alpha'\beta'}(z, \mu, q, q') \\ = \frac{i}{\hbar} [E_j(q) - E_l(q + q_0)] \eta_{jl}^{\alpha\beta}(t, x, q, q_0). \end{aligned} \quad (52)$$

We define [12]

$$T_{jm}^{\alpha\beta}(q', q) = \int_C \frac{dy}{(2\pi)^{(d-1)/2} |C|} e^{i(q' - q) \cdot y} \Phi_{m\beta}(y, q) \bar{\Phi}_{j\alpha}(y, q'). \quad (53)$$

By taking the sum over μ , the rhs becomes

$$\begin{aligned}
& \frac{1}{i\hbar} \sum_{\mu' \in L^*} \int_{\text{BZ}} \frac{dq'}{(2\pi)^d} \tilde{V}(q' + \mu') \sum_{m\alpha'\beta'} \int_{R^d} dz \left[\right. \\
& \quad (2\pi)^{(d-1)/2} T_{jm}^{\alpha\alpha'}(q, q - q' - \mu') \{u_m(t, x, q - q')\}_{\alpha'\beta'} \bar{\Phi}_{m\beta'}(z, q - q') \\
& \quad \left. - \delta_{jm} \delta_{\alpha\alpha'} \{u_m(t, x, q)\}_{\alpha'\beta'} e^{i(q' + \mu') \cdot z} \bar{\Phi}_{m\beta'}(z, q) \right] \Phi_{l\beta}(z, q + q_0) \\
& = \frac{1}{i\hbar} \sum_{\mu \in L^*} \frac{\Omega_{\text{BZ}}}{(2\pi)^{(d+1)/2}} \tilde{V}(-q_0 - \mu) \sum_{\alpha'} T_{jl}^{\alpha\alpha'}(q, q + q_0 + \mu) \{u_l(t, x, q + q_0)\}_{\alpha'\beta} \\
& \quad - \frac{1}{i\hbar} \int_{R^d} \frac{dk'}{(2\pi)^d} \tilde{V}(k') \sum_{\beta'} \{u_j(t, x, q)\}_{\alpha\beta'} \int_{R^d} dz e^{ik' \cdot z} \Phi_{l\beta}(z, q + q_0) \bar{\Phi}_{j\beta'}(z, q) \Big]. \tag{54}
\end{aligned}$$

Therefore we obtain

$$\begin{aligned}
\eta_{jl}^{\alpha\beta}(t, x, q, q_0) & = \frac{\Omega_{\text{BZ}}}{(2\pi)^{(d+1)/2}} \sum_{\mu \in L^*} \frac{\tilde{V}(-q_0 - \mu)}{E_l(q + q_0) - E_j(q) + i\xi} \\
& \times \sum_{\alpha'} \{u_l(t, x, q + q_0)\}_{\alpha'\beta} T_{jl}^{\alpha\alpha'}(q, q + q_0 + \mu) \\
& - \int_{R^{2d}} \frac{dz dk'}{(2\pi)^d} e^{ik' \cdot z} \frac{\tilde{V}(k') \sum_{\beta'} \{u_j(t, x, q)\}_{\alpha\beta'} \Phi_{l\beta}(z, q + q_0) \bar{\Phi}_{j\beta'}(z, q)}{E_l(q + q_0) - E_j(q) + i\xi}, \tag{55}
\end{aligned}$$

where ξ (> 0) is infinitesimally small.

6 Time Evolution of W_0

Next let us look at Eq. (30). We multiply $\bar{Q}_j^{\alpha\beta}(z, \mu, q)$, integrate both sides over z , and sum over μ .

$$\begin{aligned}
& \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \\
& \times \left[\frac{\partial}{\partial t} W_0 + \frac{\hbar}{m_e} \left(k + \frac{e}{\hbar} A(t, x) \right) \cdot \nabla_x W_0 - \frac{e}{m_e} \sum_{ln} \left(k_l + \frac{e}{\hbar} A_l(t, x) \right) \frac{\partial A_l(t, x)}{\partial x_n} \partial_{\mu_n} W_0 \right] \\
& = \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \\
& \times \left[\frac{\partial}{\partial t} W_0 + \sum_l \left(k_l + \frac{e}{\hbar} A_l(t, x) \right) \left(\frac{\hbar}{m_e} \frac{\partial}{\partial x_l} - \frac{e}{m_e} A_l(t, \nabla_\mu) \right) W_0 \right] \\
& = - \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \left[\mathcal{L} W_2 + \frac{i\hbar}{m_e} \nabla_x \cdot \nabla_z W_0 \right]
\end{aligned}$$

$$\begin{aligned}
& + \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \\
& \times \frac{1}{i\hbar} \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \hat{V}(k') [W_1(t, x, z, k - k') - W_1(t, x, z, k)].
\end{aligned} \tag{56}$$

The first integral on the rhs vanishes (\mathcal{L} is skew symmetric and $Q_j^{\alpha\beta} \in \ker \mathcal{L}$).

6.1 LHS

The lhs of Eq. (56) is calculated as follows. The first term is easy.

$$\begin{aligned}
& \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \frac{\partial}{\partial t} W_0 \\
& = \sum_{m, \alpha', \beta'} \frac{\partial}{\partial t} \{u_m(t, x, q)\}_{\alpha' \beta'} \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) Q_m^{\alpha' \beta'}(z, \mu, q) \\
& = \frac{\partial}{\partial t} \{u_j(t, x, q)\}_{\alpha \beta}.
\end{aligned} \tag{57}$$

The second term is calculated as follows.

$$\begin{aligned}
& \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \left(k_l + \frac{e}{\hbar} A_l(x)\right) \left(\frac{\partial}{\partial x_l} - \frac{e}{\hbar} A_l(\nabla_\mu)\right) \\
& \times \{u_m(t, x, q)\}_{\alpha' \beta'} Q_m^{\alpha' \beta'}(z, \mu, q) \\
& = \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \int_C \frac{dy'}{|C|} \left[\left(-i \frac{\partial}{\partial y'_l} + \frac{e}{\hbar} A_l(x)\right) e^{i(q+\mu) \cdot y'} \right] \\
& \times \left\{ \frac{\partial u_m}{\partial x_l} - \frac{ie}{\hbar} u_m A_l(y') \right\}_{\alpha' \beta'} \Phi_{m\alpha'}(z - y', q) \bar{\Phi}_{m\beta'}(z, q). \\
& = \frac{\partial \{u_j\}_{\alpha' \beta'}}{\partial x_l} \delta_{jm} \delta_{\beta \beta'} \left[-i \left(\frac{\partial \Phi_{j\alpha'}}{\partial z_l}, \Phi_{j\alpha} \right) + \frac{e}{\hbar} A_l(x) \delta_{\alpha \alpha'} \right] \\
& - \frac{ie}{\hbar} \{u_m\}_{\alpha' \beta'} \left[-i \left(\frac{\partial \Phi_{m\alpha'}}{\partial z_l}, \Phi_{j\alpha} \right) (A_l \Phi_{j\beta}, \Phi_{m\beta'}) + \frac{e}{\hbar} A_l(x) \delta_{jm} \delta_{\alpha \alpha'} (A_l \Phi_{j\beta}, \Phi_{m\beta'}) \right. \\
& \left. + i \delta_{jm} \delta_{\beta \beta'} \left(A_l \frac{\partial \Phi_{m\alpha'}}{\partial z_l}, \Phi_{j\alpha} \right) - \delta_{jm} \delta_{\beta \beta'} \frac{e}{\hbar} A_l(x) (A_l \Phi_{m\alpha'}, \Phi_{j\alpha}) \right].
\end{aligned} \tag{58}$$

Therefore, the lhs of Eq. (56) is written as

$$\begin{aligned}
& \frac{\partial}{\partial t} \{u_j(t, x, q)\}_{\alpha \beta} + \frac{1}{\hbar} \nabla_q E_j(q) \cdot \nabla_x \{u_j(t, x, q)\}_{\alpha \beta} + \frac{e}{\hbar} \\
& \times \left[\sum_{\alpha'} \left(\frac{i}{\hbar} \nabla_q E_j \cdot A(z) \Phi_{j\alpha'}(z), \Phi_{j\alpha}(z) \right) \{u_j(t, x, q)\}_{\alpha' \beta} \right. \\
& \left. - \sum_{\beta'} \{u_j(t, x, q)\}_{\alpha \beta'} \left(\frac{i}{\hbar} \nabla_q E_j \cdot A(z) \Phi_{j\beta}(z), \Phi_{j\beta'}(z) \right) \right].
\end{aligned} \tag{59}$$

6.2 RHS

Let us calculate the rhs of Eq. (56). After taking ensemble average, the rhs is given by the sum of two matrices I_1 and I_2 where

$$\{I_1\}_{\alpha\beta} = \frac{1}{i\hbar} \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \times \langle \tilde{V}(k') W_1(t, x, z, k - k') \rangle, \quad (60)$$

$$\{I_2\}_{\alpha\beta} = -\frac{1}{i\hbar} \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \times \langle \tilde{V}(k') W_1(t, x, z, k) \rangle. \quad (61)$$

Using Eq. (51) and Eq. (55), I_1 is written as

$$I_1 = I_{11} - I_{12}, \quad (62)$$

where

$$\begin{aligned} \{I_{11}\}_{\alpha\beta} &= \frac{1}{i\hbar} \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \sum_{mn\alpha'\beta'} \int_{\text{BZ}} \frac{dq''}{\Omega_{\text{BZ}}} \\ &\times \frac{\Omega_{\text{BZ}}}{(2\pi)^{(d+1)/2}} \sum_{\mu'' \in L^*} \frac{\langle \tilde{V}(k') \tilde{V}(-q'' - \mu'') \rangle}{E_n(q - q' + q'') - E_m(q - q') + i\xi} \\ &\times \sum_{\alpha''} \{u_n(t, x, q - q' + q'')\}_{\alpha''\beta'} T_{mn}^{\alpha'\alpha''}(q - q', q - q' + q'' + \mu'') \\ &\times P_{mn}^{\alpha'\beta'}(z, \mu - \mu', q - q', q''), \end{aligned} \quad (63)$$

and

$$\begin{aligned} \{I_{12}\}_{\alpha\beta} &= \frac{1}{i\hbar} \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta}(z, \mu, q) \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \sum_{mn\alpha'\beta'} \int_{\text{BZ}} \frac{dq''}{\Omega_{\text{BZ}}} \\ &\times \int_{R^{2d}} \frac{dz' dk_1}{(2\pi)^d} e^{ik_1 \cdot z'} \langle \tilde{V}(k') \tilde{V}(k_1) \rangle P_{mn}^{\alpha'\beta'}(z, \mu - \mu', q - q', q'') \\ &\times \frac{\sum_{\beta''} \{u_m(t, x, q - q')\}_{\alpha'\beta''} \Phi_{n\beta'}(z', q - q' + q'') \bar{\Phi}_{m\beta''}(z', q - q')}{E_n(q - q' + q'') - E_m(q - q') + i\xi}. \end{aligned} \quad (64)$$

We obtain

$$\begin{aligned} \{I_{11}\}_{\alpha\beta} &= \frac{1}{i\hbar} \sum_m \sum_{\mu'' \in L^*} \int_{\text{BZ}} \frac{dq''}{2\pi} \frac{\tilde{R}(-q'' - \mu'')}{E_j(q) - E_m(q - q'') + i\xi} \sum_{\alpha'\alpha''} \{u_j(t, x, q)\}_{\alpha''\beta} \\ &\times T_{mj}^{\alpha'\alpha''}(q - q'', q + \mu'') T_{jm}^{\alpha\alpha'}(q + \mu'', q - q''). \end{aligned} \quad (65)$$

Similarly we also obtain I_{12} .

$$\begin{aligned} \{I_{12}\}_{\alpha\beta} &= \frac{1}{i\hbar} \int_{R^d} \frac{dk'}{2\pi} \sum_m \frac{\tilde{R}(-k')}{E_j(q) - E_m(q - q') + i\xi} \\ &\quad \times \sum_{\alpha'\beta''} \{u_m(t, x, q - q')\}_{\alpha'\beta''} T_{jm}^{\alpha\alpha'}(q, q - k') T_{mj}^{\beta''\beta}(q - k', q), \end{aligned} \quad (66)$$

where we used

$$\int_{R^d} dz' = \sum_{v \in L} \int_C dy, \quad \frac{1}{\Omega_{\text{BZ}}} \sum_{v \in L} e^{iq \cdot v} = \sum_{\mu \in L^*} \delta(q + \mu). \quad (67)$$

We have

$$\begin{aligned} \{I_1\}_{\alpha\beta} &= \frac{1}{i\hbar} \sum_m \sum_{\mu' \in L^*} \int_{\text{BZ}} \frac{dq'}{2\pi} \frac{\tilde{R}(-q' - \mu')}{E_j(q) - E_m(q - q') + i\xi} \left[\right. \\ &\quad \sum_{\alpha'\alpha''} T_{jm}^{\alpha\alpha'}(q, q - q' - \mu') T_{mj}^{\alpha'\alpha''}(q - q' - \mu', q) \{u_j(t, x, q)\}_{\alpha''\beta} \\ &\quad \left. - \sum_{\alpha'\beta''} T_{jm}^{\alpha\alpha'}(q, q - q' - \mu') \{u_m(t, x, q - q')\}_{\alpha'\beta''} T_{mj}^{\beta''\beta}(q - q' - \mu', q) \right]. \end{aligned} \quad (68)$$

In the same way, we have

$$\begin{aligned} \{I_2\}_{\alpha\beta} &= \frac{-1}{i\hbar} \sum_n \sum_{\mu' \in L^*} \int_{\text{BZ}} \frac{dq'}{2\pi} \frac{\tilde{R}(-q' - \mu')}{E_n(q + q') - E_j(q) + i\xi} \left[\right. \\ &\quad \sum_{\alpha''\beta'} T_{jn}^{\alpha\alpha''}(q, q + q' + \mu') \{u_n(t, x, q + q')\}_{\alpha''\beta'} T_{nj}^{\beta'\beta}(q + q' + \mu', q) \\ &\quad \left. - \sum_{\beta'\beta''} \{u_j(t, x, q)\}_{\alpha\beta''} T_{jn}^{\beta''\beta'}(q, q + q' + \mu') T_{nj}^{\beta'\beta}(q + q' + \mu', q) \right]. \end{aligned} \quad (69)$$

Thus we see the relation

$$I_2 = I_1^*, \quad (70)$$

where $*$ denotes the Hermitian conjugate. By summing I_1 and I_2 , and using the relation

$$\bar{T}_{mj}^{\beta\alpha}(q, q') = T_{jm}^{\alpha\beta}(q', q), \quad (71)$$

the rhs of Eq. (56) becomes

$$\begin{aligned} I_1 + I_1^* &= \frac{1}{i\hbar} \sum_m \sum_{\mu' \in L^*} \int_{\text{BZ}} \frac{dq'}{2\pi} \tilde{R}(-q' - \mu') \left[\right. \\ &\quad T_{jm}(q, q - q' - \mu') u_m(t, x, q - q') T_{mj}(q - q' - \mu', q) \end{aligned}$$

$$\begin{aligned}
& \times \left(\frac{1}{E_j(q) - E_m(q - q') - i\xi} - \frac{1}{E_j(q) - E_m(q - q') + i\xi} \right) \\
& + \frac{T_{jm}(q, q - q' - \mu') T_{jm}^*(q, q - q' - \mu') u_j(t, x, q)}{E_j(q) - E_m(q - q') + i\xi} \\
& - \frac{u_j(t, x, q) T_{jm}(q, q - q' - \mu') T_{jm}^*(q, q - q' - \mu')}{E_j(q) - E_m(q - q') - i\xi} \Big]. \tag{72}
\end{aligned}$$

We change the variable as $q' \rightarrow q - q'$ and obtain

$$\begin{aligned}
I_1 + I_1^* &= \frac{1}{i\hbar} \sum_m \sum_{\mu' \in L^*} \int_{\text{BZ}} \frac{dq'}{2\pi} \tilde{R}(-q' - \mu') \left[\right. \\
& 2\pi i T_{jm}(q, q' - \mu') u_m(t, x, q') T_{mj}(q' - \mu', q) \delta(E_j(q) - E_m(q')) \\
& + \frac{T_{jm}(q, q' - \mu') T_{jm}^*(q, q' - \mu') u_j(t, x, q)}{E_j(q) - E_m(q') + i\xi} \\
& \left. - \frac{u_j(t, x, q) T_{jm}(q, q' - \mu') T_{jm}^*(q, q' - \mu')}{E_j(q) - E_m(q') - i\xi} \right]. \tag{73}
\end{aligned}$$

6.3 Radiative Transport Equation

We define a vector $v_j(q)$, a matrix $M_j(q)$, and a superoperator $\hat{\mu}_L$ as

$$v_j(q) = \frac{1}{\hbar} \nabla_q E_j(q), \tag{74}$$

$$\{M_j(q)\}_{\alpha\beta} = \left(\frac{ie}{\hbar} v_j(q) \cdot A \Phi_{j\beta}, \Phi_{j\alpha} \right), \tag{75}$$

$$\hat{\mu}_L : u_j(q) \mapsto [M_j(q), u_j(q)] = M_j(q) u_j(q) - u_j(q) M_j(q). \tag{76}$$

Furthermore let us define the following superoperators.

$$\begin{aligned}
\hat{A}(q, q') : u_j(q_0) &\mapsto \frac{1}{\hbar} \sum_m \sum_{\mu' \in L^*} \tilde{R}(-q' - \mu') \delta(E_j(q) - E_m(q')) \\
& T_{jm}(q, q' - \mu') u_m(q_0) T_{mj}(q' - \mu', q), \tag{77}
\end{aligned}$$

$$\begin{aligned}
\hat{\mu}_s : u_j(q) &\mapsto \frac{-1}{i\hbar} \sum_m \sum_{\mu' \in L^*} \int_{\text{BZ}} \frac{dq'}{2\pi} \tilde{R}(-q' - \mu') \\
& \left[\frac{T_{jm}(q, q' - \mu') T_{jm}^*(q, q' - \mu') u_j(q)}{E_j(q) - E_m(q') + i\xi} \right. \\
& \left. - \frac{u_j(q_0) T_{jm}(q, q' - \mu') T_{jm}^*(q, q' - \mu')}{E_j(q) - E_m(q') - i\xi} \right]. \tag{78}
\end{aligned}$$

Finally, by Eqs. (30), (56), (59), and (73), we obtain the RTE as

$$\begin{aligned} \frac{\partial}{\partial t} u_j(t, x, q) + v_j(q) \cdot \nabla_x u_j(t, x, q) + (\hat{\mu}_L + \hat{\mu}_s) u_j(t, x, q) \\ = \int_{\text{BZ}} dq' \hat{A}(q, q') u_j(t, x, q'). \end{aligned} \quad (79)$$

Note that the term for $\hat{\mu}_L$ stems from the Lorentz force. The terms for $\hat{\mu}_s$ and \hat{A} stem from the random potential.

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